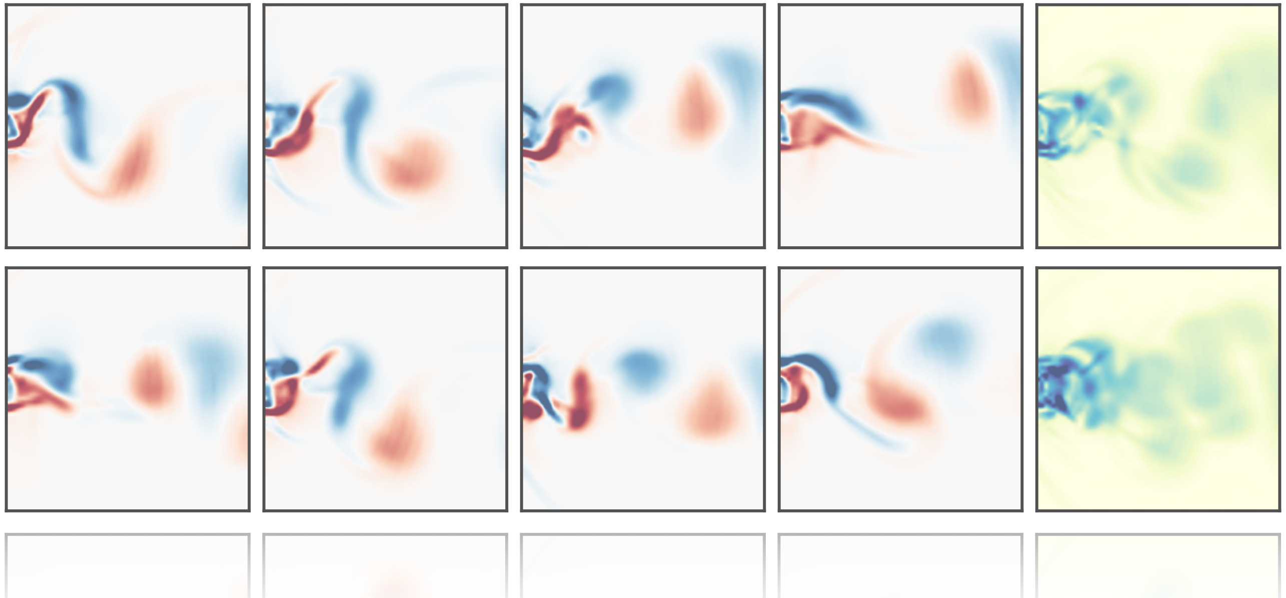


Differentiable Physics Simulations for Deep Learning

(… from a Diffusion Modeling Perspective)

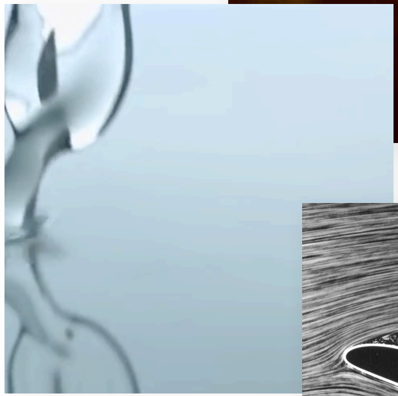
Nils Thuerey

Introduction

- Growing consensus: DL is “just” another tool
- … but a pretty neat one
- Unclear how / where to employ

Introduction

- Important to work with uncertainties in simulations
  - Inherent randomness of processes & ambiguous states (*aleatoric*)
  - Model approximations and errors (*epistemic*)
- Here: dealing with aleatoric uncertainties with the help of *deep learning* algorithms and *differentiable* simulations

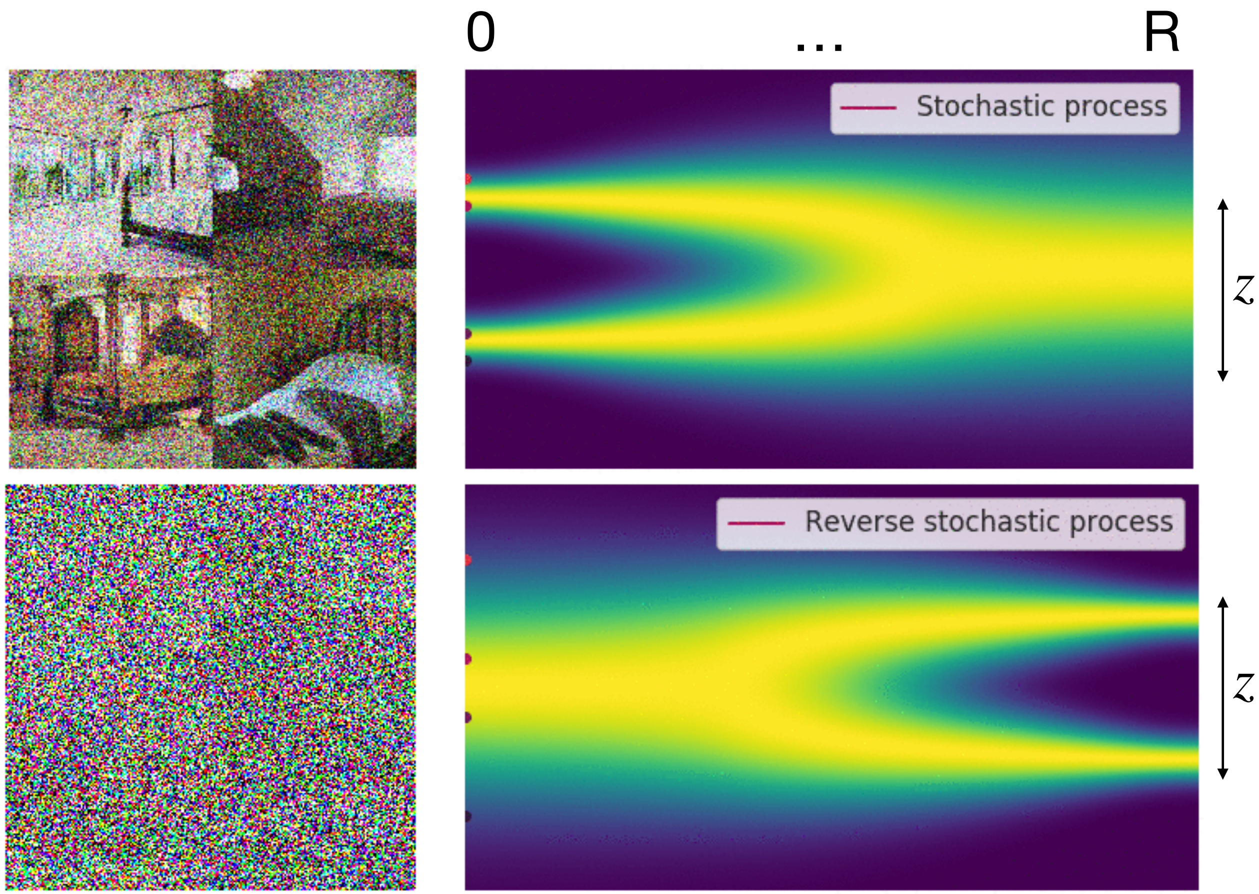




Diffusion Models

- Quantity of interest $\bar{y} = f(x)$, approximated by NN with weights θ: $y = f_\theta(x) \approx \bar{y}$
- Optimize θ via arg min$_\theta | \bar{y} - f_\theta(x) |_2$
- *Denoising diffusion probabilistic models* (DDPMs) introduce Markov chain with steps $r \in 0,\ldots,R$ with increasing Gaussian noise
- Learn reverse process $y_{r-1} = \alpha y_r + \beta\, f_\theta(y_r, x, r) + z$ such that $y_0 \approx \bar{y}$
- α, β are factors determined by noise schedule and $z \sim \mathcal{N}(0,1)$

Diffusion Models

- Illustrated:



Generate data from noise by reversing the perturbation procedure. Source: https://yang-song.net/blog/2021/score/

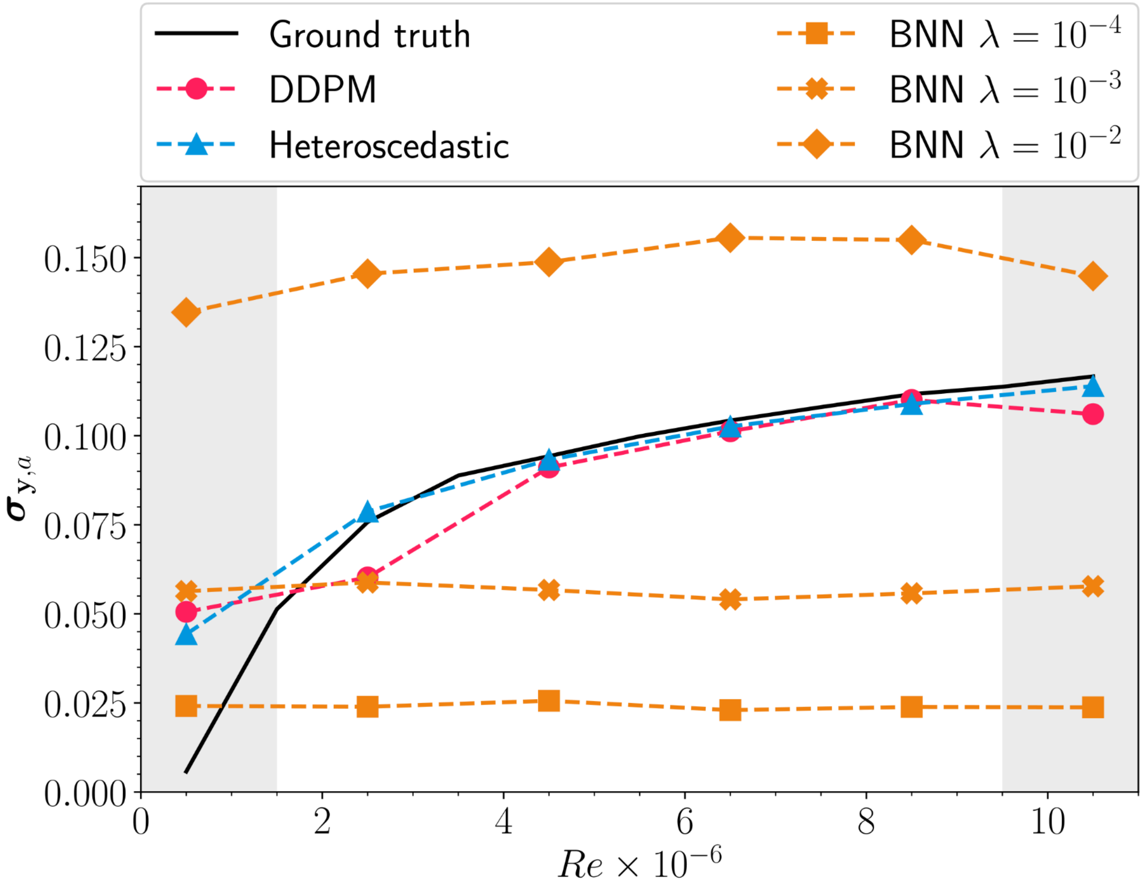
Known Ground Truth Distribution

- Turbulent NS case with varying Reynolds number:

- *Heteroscedastic model (blue)* works but no posterior samples

- *Bayesian NN (orange)* fares badly

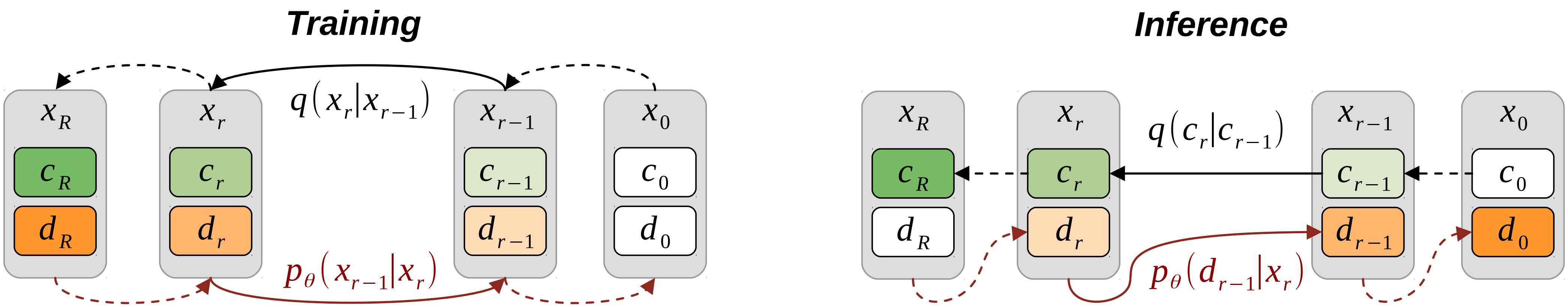
- *DDPM (red)* captures ground truth distribution and can produce actual samples…



Liu et. al: Uncertainty of Turbulence Simulations with Denoising Diffusion Probabilistic Models

Diffusion Models for Temporal Processes

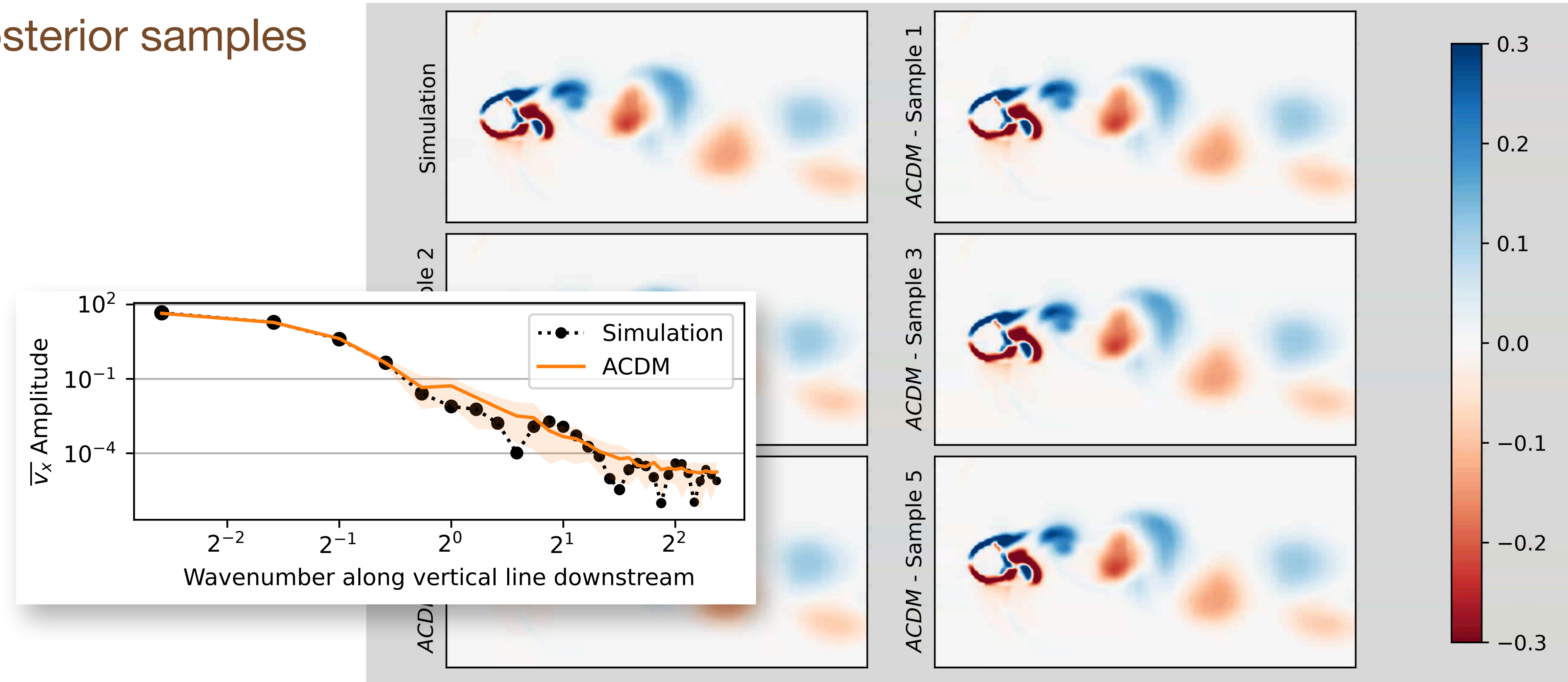
- Temporal stability crucial (iterative / auto-regressive / unrolled predictions)
- Diffusion models also pay off in this context
- Important: conditioning on previous state and global parameters



Kohl *et. al*: Turbulent Flow Simulation using Autoregressive Conditional Diffusion Models

Transonic Flow Example

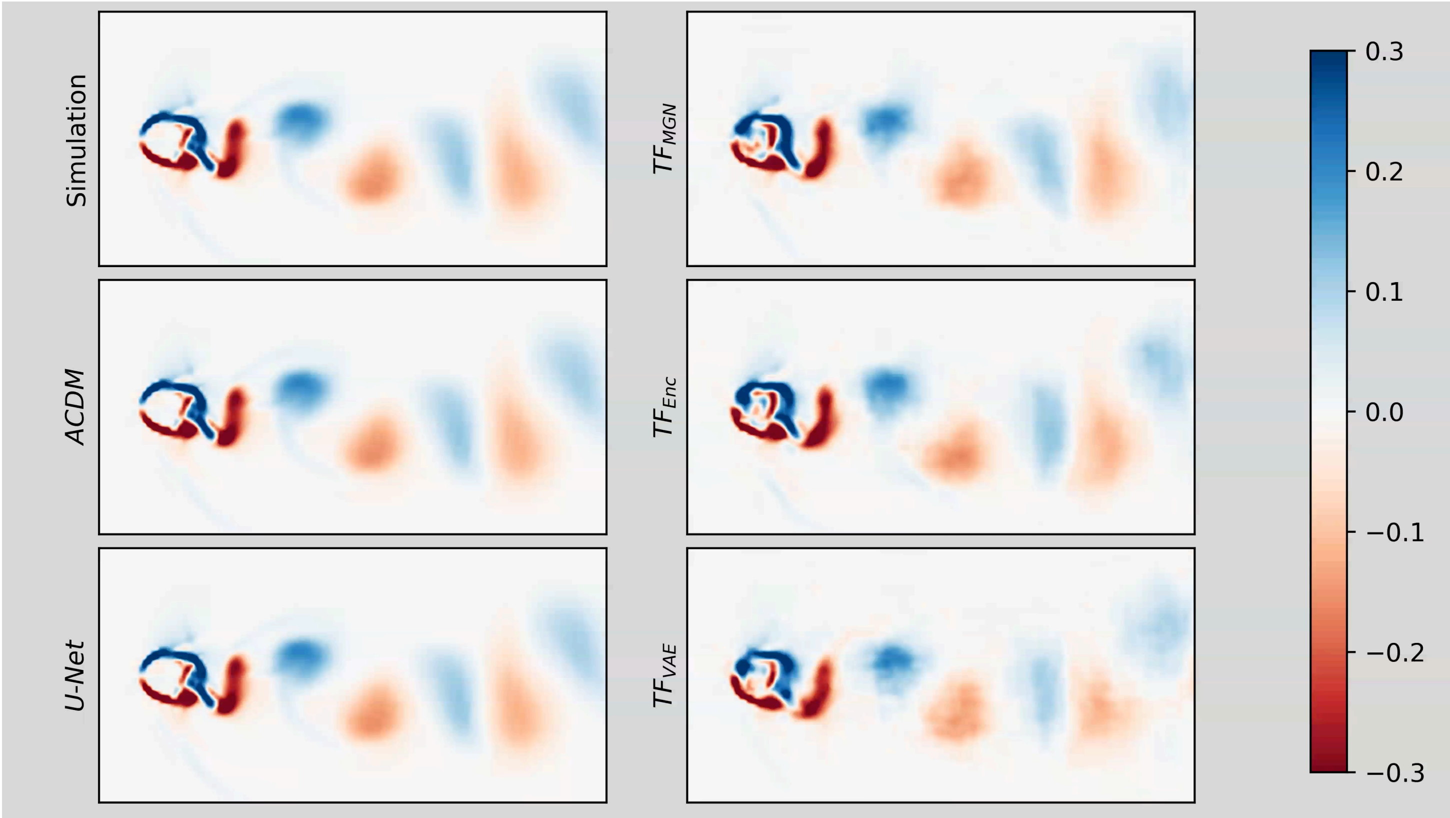
- Posterior samples



Kohl *et. al*: Turbulent Flow Simulation using Autoregressive Conditional Diffusion Models

Transonic Flow Example

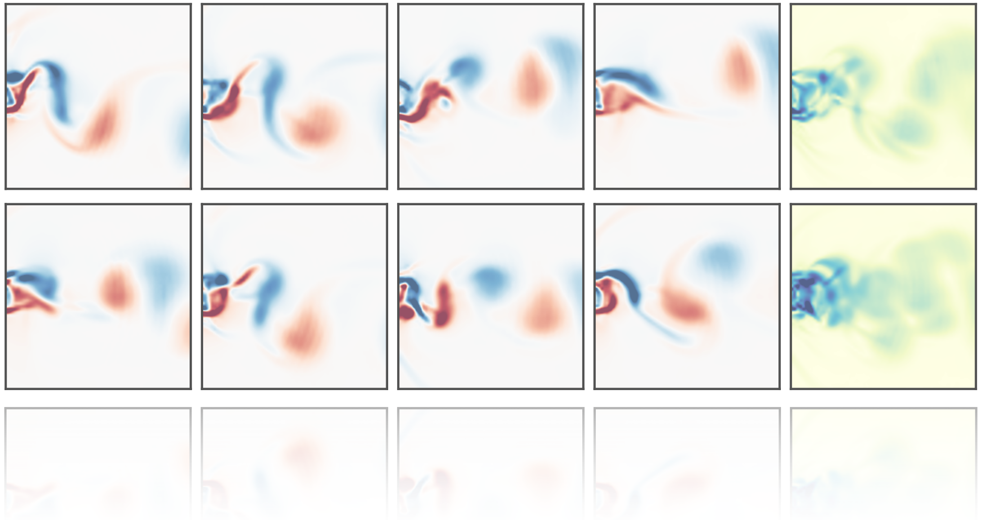
- Versus baselines: simple *U-net* , and SOTA *transformer.*



Kohl *et. al*: Turbulent Flow Simulation using Autoregressive Conditional Diffusion Models

Diffusion Models for Temporal Processes

- Summary so far:
  - Excellent temporal stability
  - Enable posterior sampling
  - Increased computational cost



Kohl *et. al*: Turbulent Flow Simulation using Autoregressive Conditional Diffusion Models

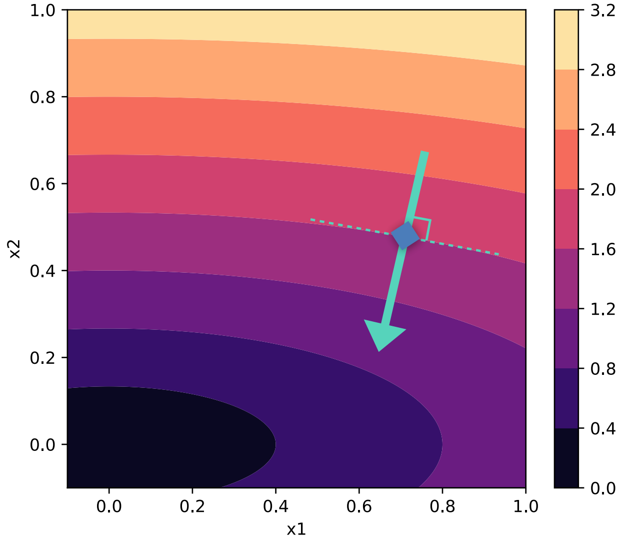
Differentiable Simulations in a Nutshell

Discretized PDE $\mathscr{P}$ with phase space states $\mathbf{s}$

Learn via gradient $(\partial\mathscr{P}/\partial\mathbf{s})^T$

E.g., with loss L and $\mathbf{s} = \mathrm{NN}(\mathbf{x}\,|\,\theta)$

Gradient is $-\eta \dfrac{\partial \mathbf{s}}{\partial \theta}^T \dfrac{\partial \mathscr{P}}{\partial \mathbf{s}}^T \dfrac{\partial L}{\partial \mathscr{P}}^T$



Requires differentiable physics simulator for $\mathscr{P}$

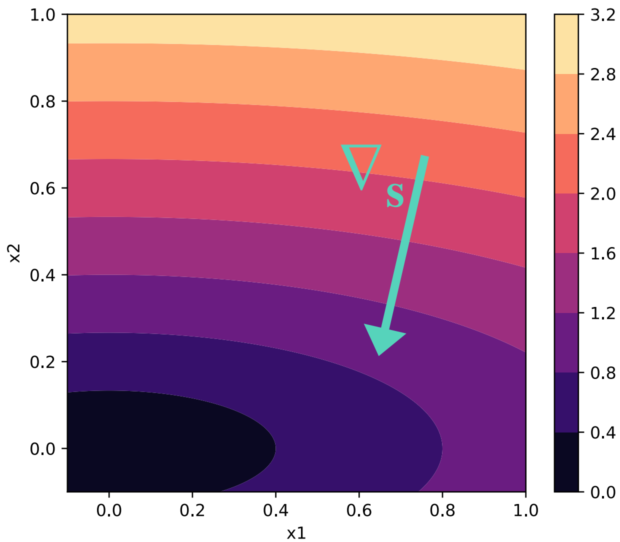
→ Tight integration of numerical methods and learning process

Differentiable Simulations - Terminology

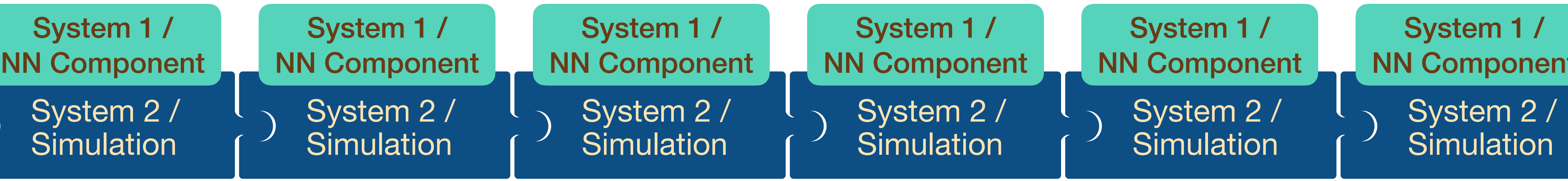
Differentiable PDE solver for $\mathscr{P}$ = "differentiable physics"

Equivalent:

- *Adjoint method / differentiation*
- *Reverse-mode / backward differentiation*
- *Backpropagation*

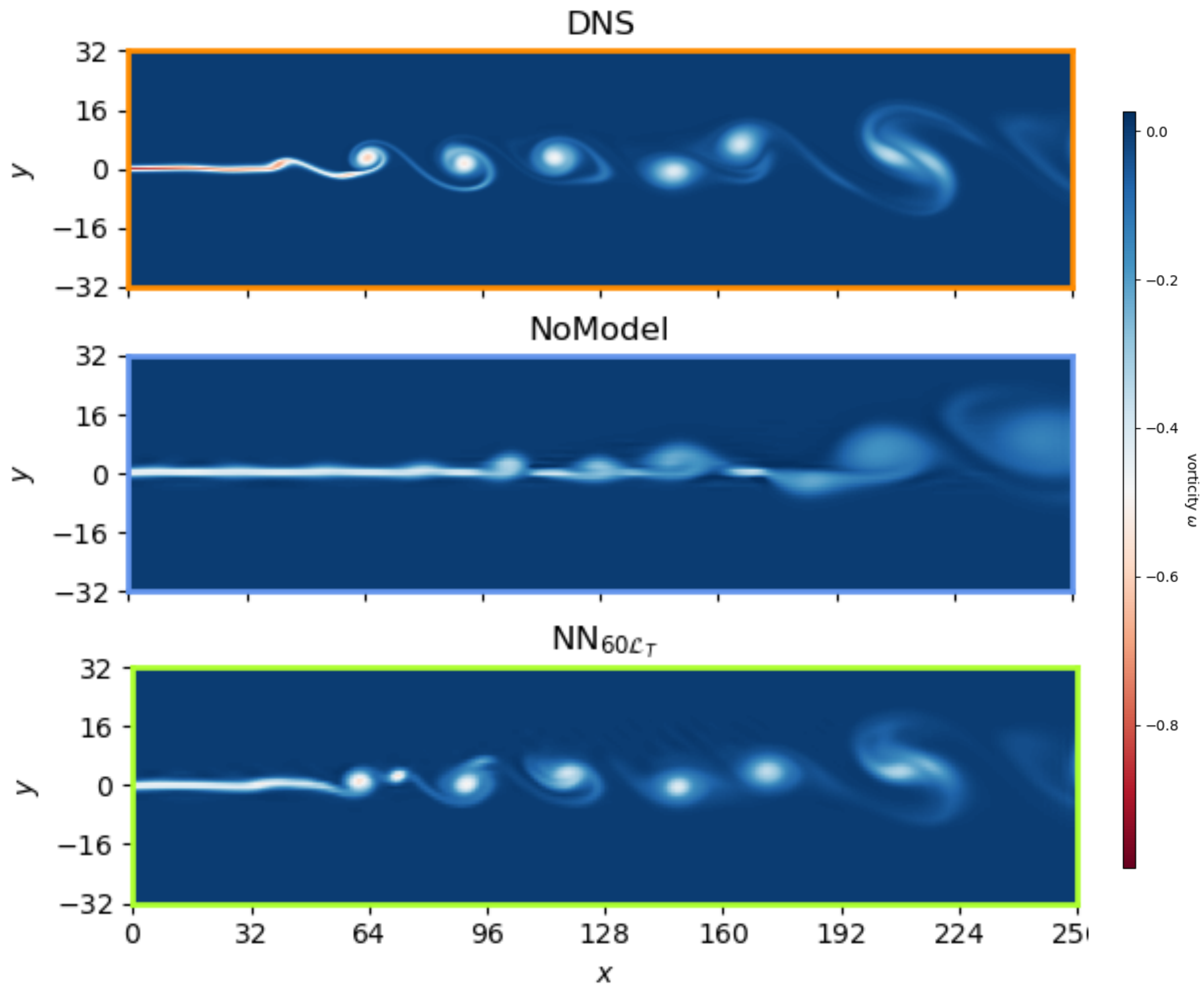


D. Kahneman: System 1 & 2



Turbulence: Spatial Mixing Layer

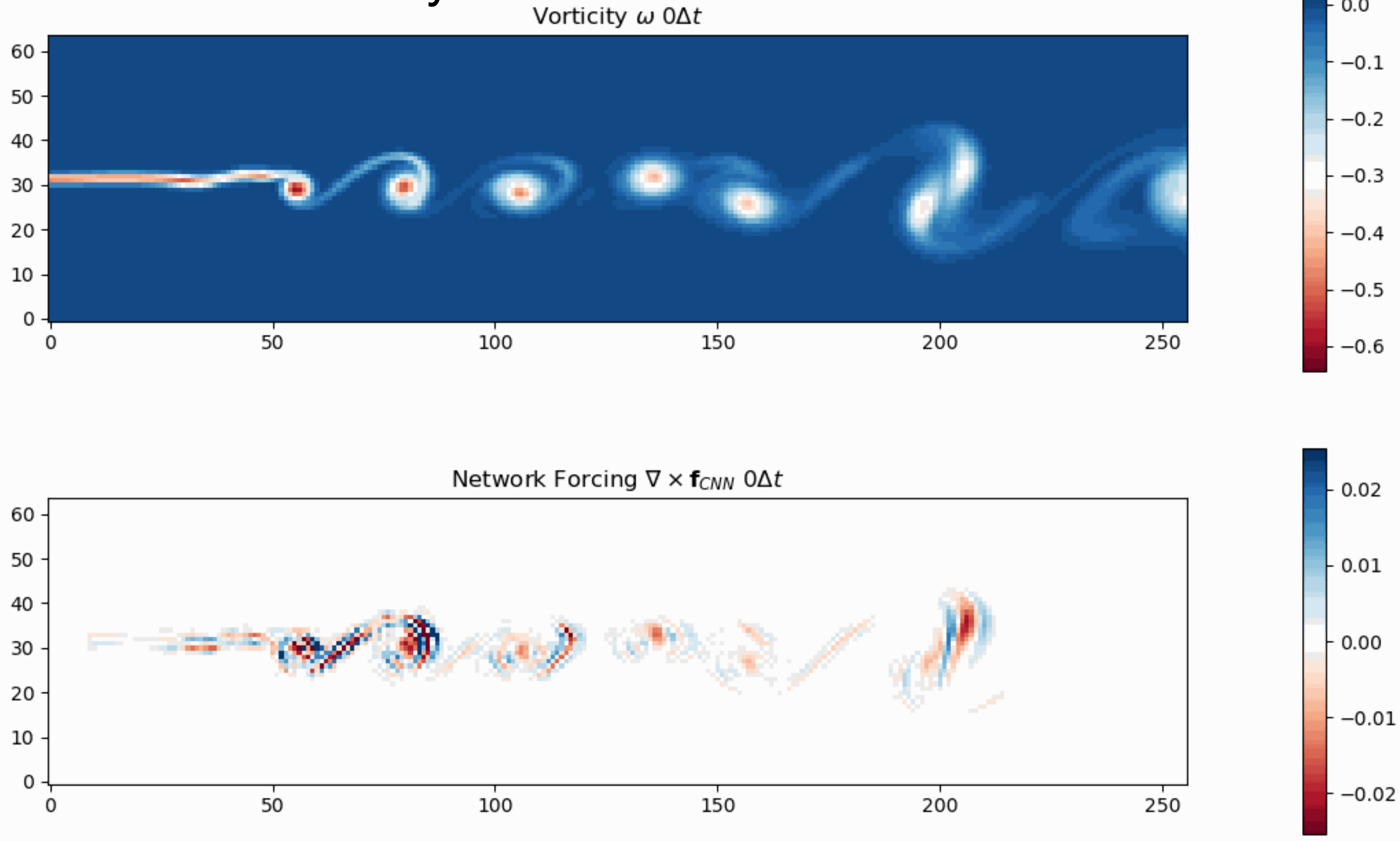
- Semi-implicit PISO solver (2nd order in time)
- Shear layer with vorticity thickness Re = 500
- Evaluate on test set of unseen perturbation modes



List et. al: Learned Turbulence Modelling with Differentiable Fluid Solvers

Turbulence: Spatial Mixing Layer

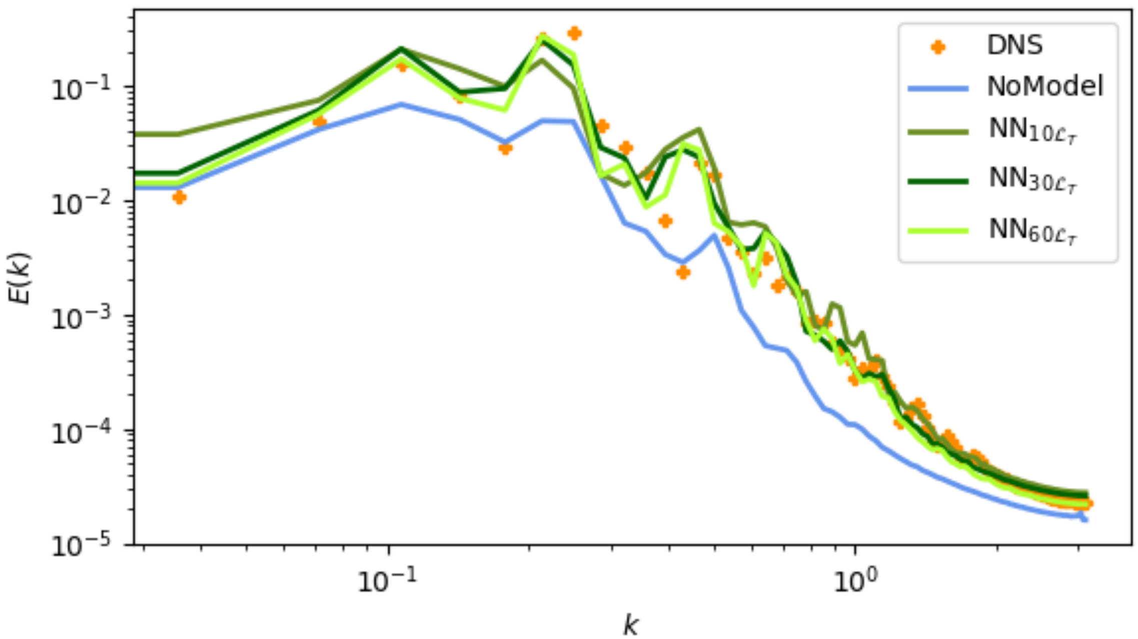
Learned Simulator only:



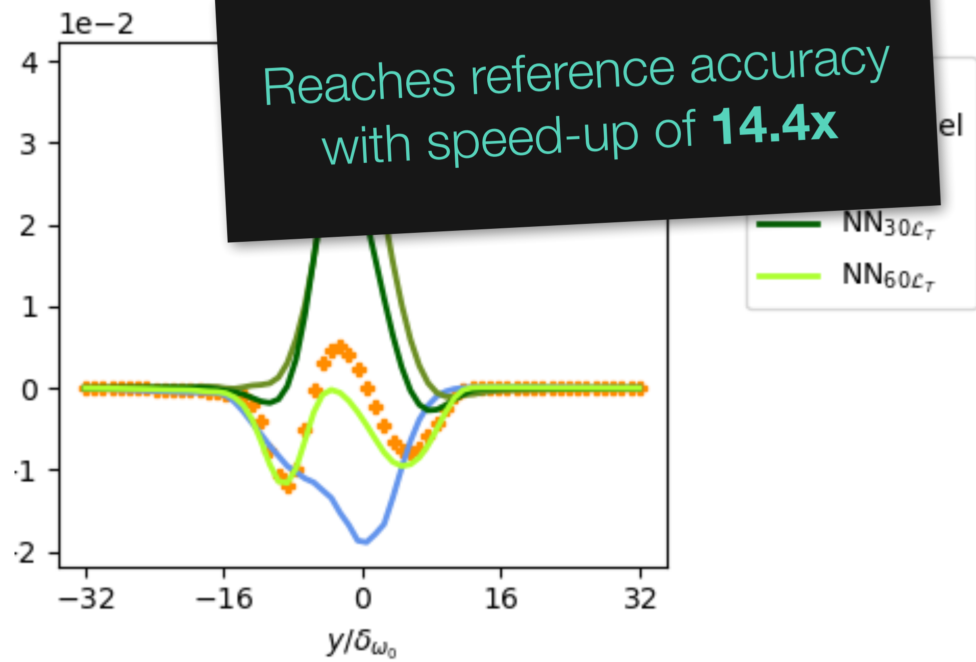
List et. al: Learned Turbulence Modelling with Differentiable Fluid Solvers

Turbulence: Spatial Mixing Layer

Closely matches DNS turbulence statistics (steady state over 2500 steps)



Energy spectrum



Reynolds stresses

Reaches reference accuracy with speed-up of **14.4x**

List et. al: Learned Turbulence Modelling with Differentiable Fluid Solvers

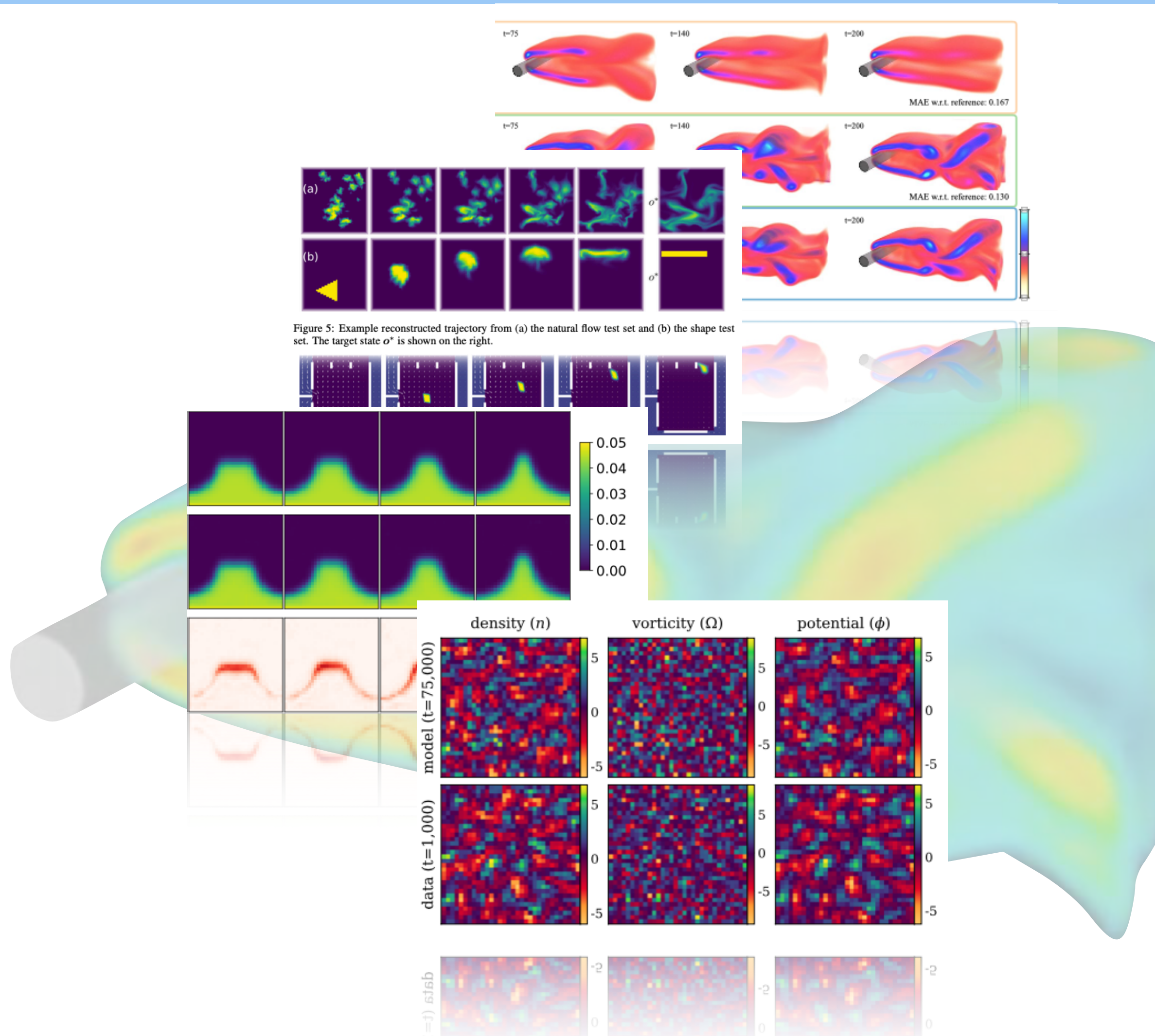
Differentiable Simulations

Successfully applied to:

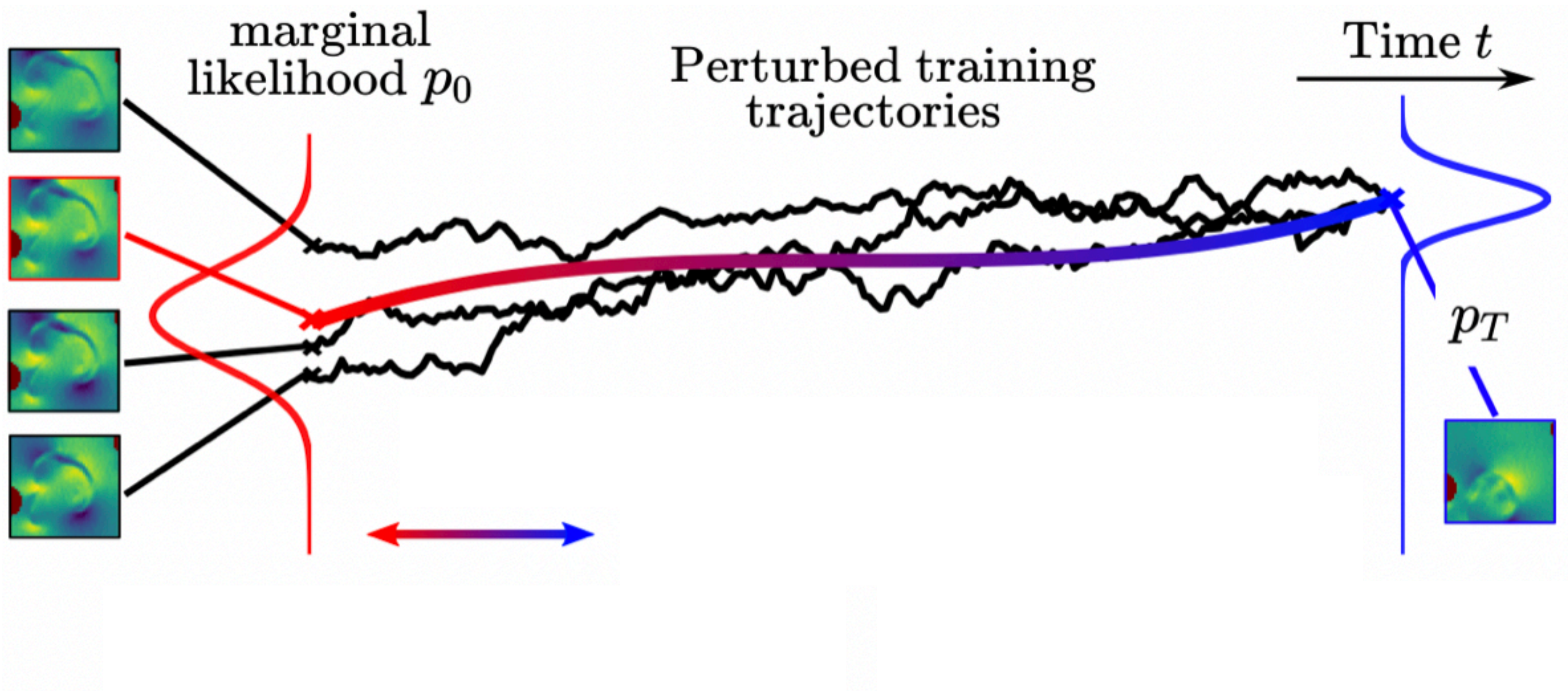
[- Turbulence]

- Control problems
- Chemical reactions
- Plasma simulations
- …

→ Also attractive for diffusion models



Diffusion Models for Physics Simulations



Holzschuh et. al: Solving Inverse Physics Problems with Score Matching

Diffusion Models for Physics Simulations

Forward evolution via Euler-Maruyama:

$$\mathbf{x}_{t+\Delta t} \approx \mathbf{x}_t + \Delta t\, \mathscr{P}(\mathbf{x}_t) + \sqrt{\Delta t}\, g(t)\, z_t \quad \text{with } z_t \sim \mathcal{N}(0, I)$$

Reverse time SDE via score matching formulation:

$$\mathbf{x}_t \approx \mathbf{x}_{t+\Delta t} - \Delta t \left[\mathscr{P}(\mathbf{x}_{t+\Delta t}) + g^2(t+\Delta t)\, \nabla_{\mathbf{x}} \log p_{t+\Delta t}(\mathbf{x}_{t+\Delta t}) \right] + \sqrt{\Delta t}\, g(t+\Delta t)\, \tilde{z}_{t+\Delta t}$$

Differentiable physics simulator , learned score (“correction”)

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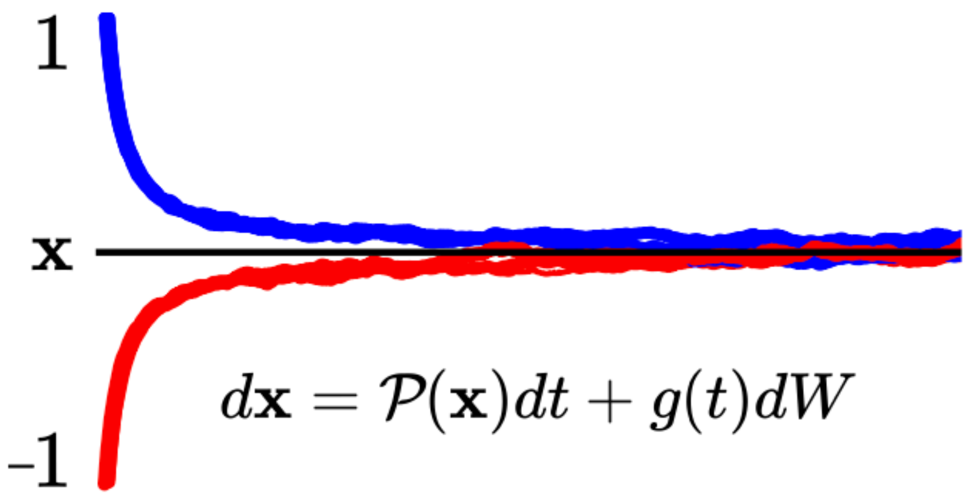
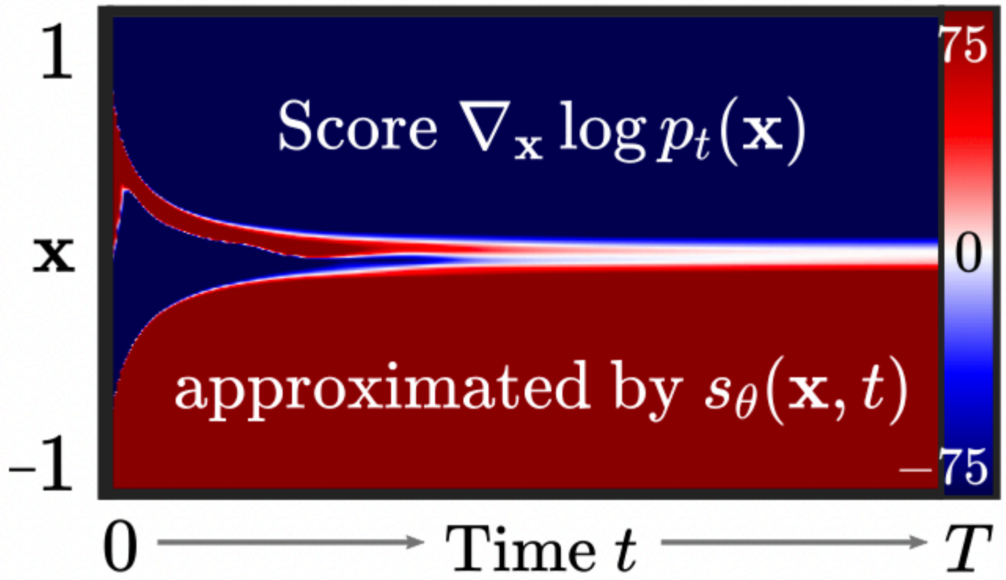
1D Example

Toy problems: randomized sign function





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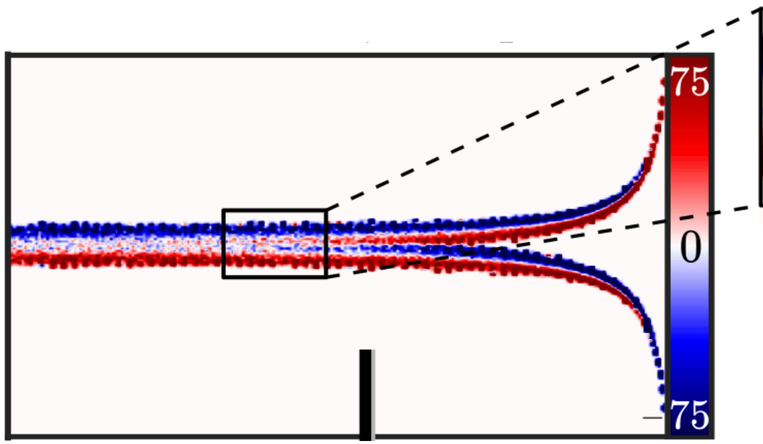
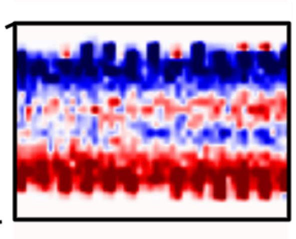
1D Example

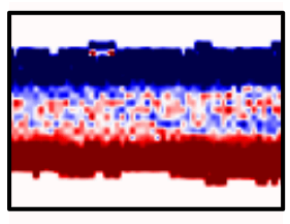
As before, train with back-propagation through multiple simulation steps:





1-Step training:

Noisy & unreliable



Multi-step:

Improved consistence

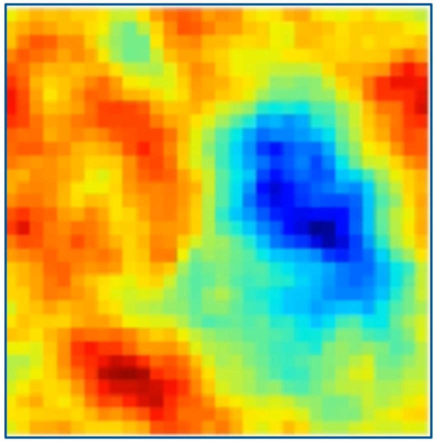
→ Exploding trajectories

→ Stable

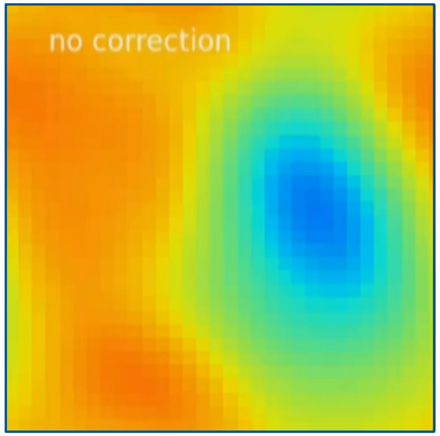
Heat Diffusion Case

Heat equation $\frac{\partial u}{\partial t} = \alpha \Delta u$ with $\alpha = 1$, Gaussian random fields as initial conditions

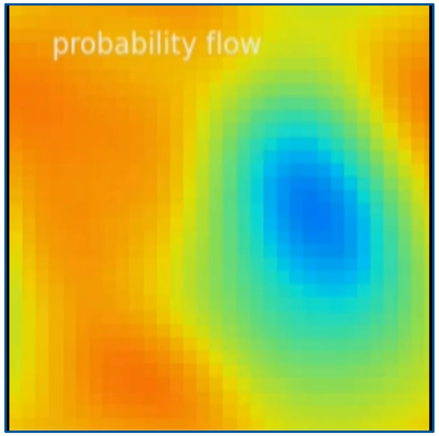
Ground truth at $t = 0.0$



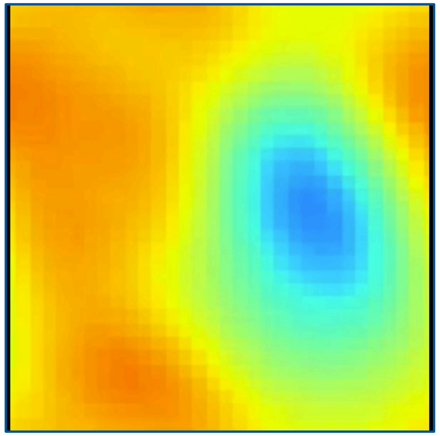
$\tilde{\mathscr{P}}^{-1}$ only



Probability flow



Reverse-time SDE



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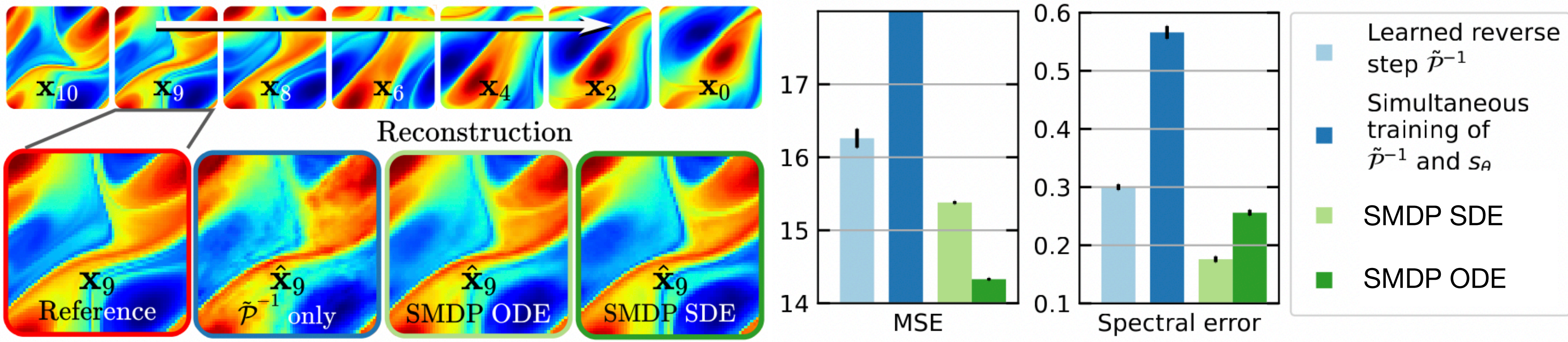
Navier-Stokes Case

Isotropic turbulence with pre-trained surrogate simulator:

Reconstructed trajectories

Evaluation



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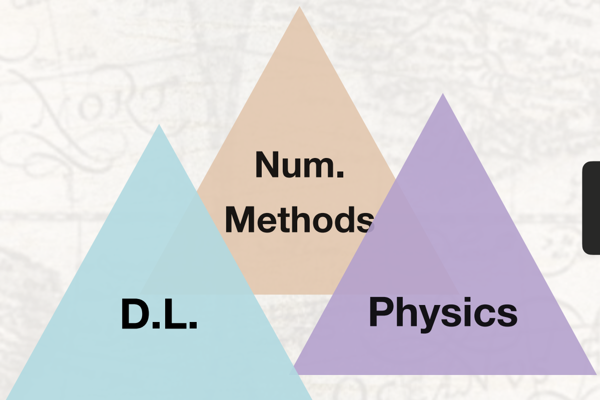
Summary & Outlook

Summary

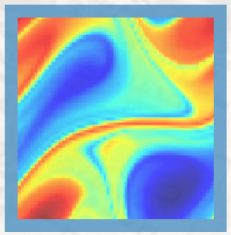
Differentiable Simulations and Diffusion Models

as Tools to bridge Physics & Learning 🤗

Deep Learning

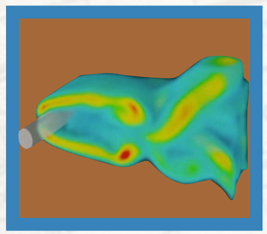


Physical Systems



Score Matching

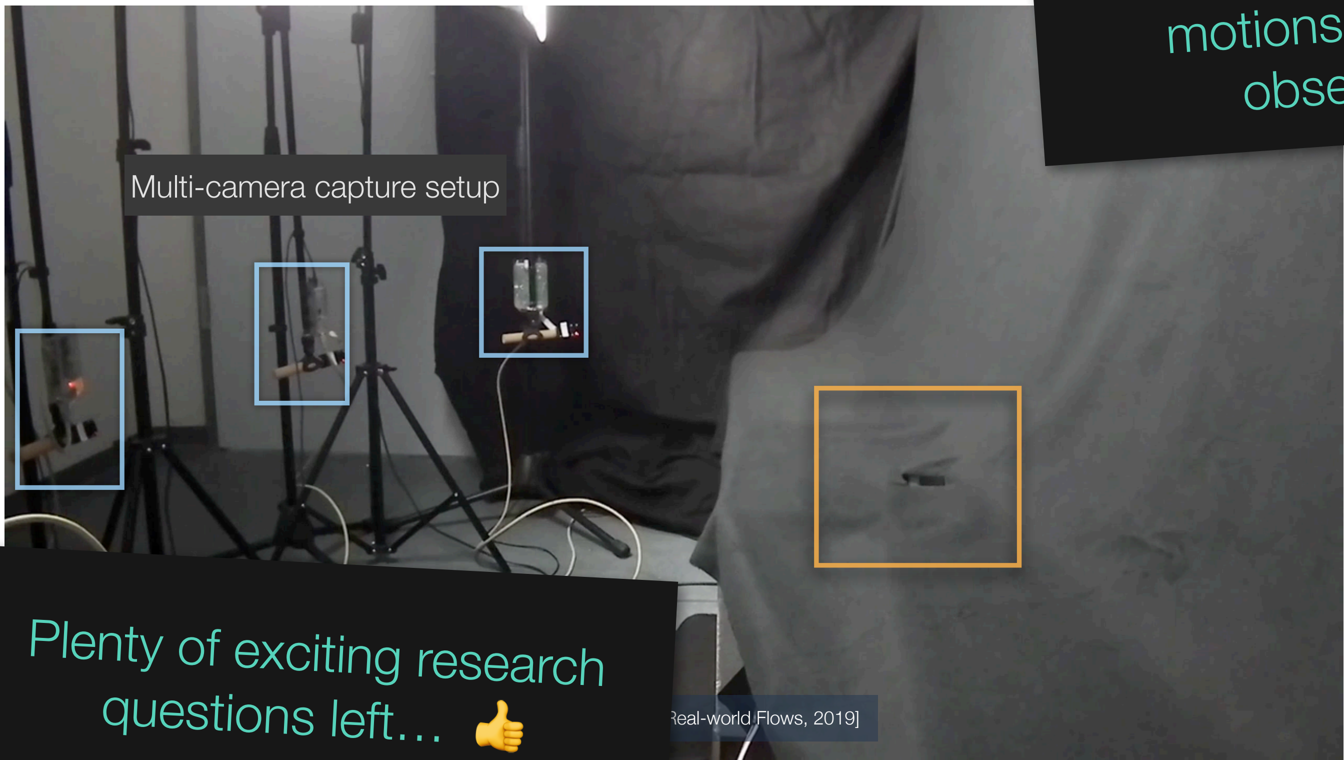
Turbulence Modeling

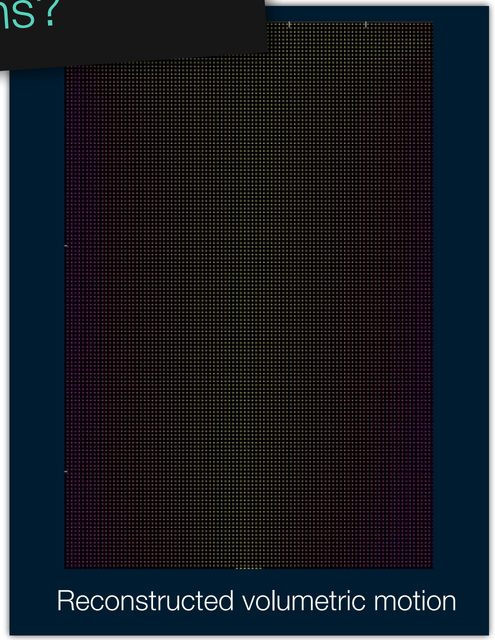


Time Predictions

Learn from Real-world Observations

Reconstruct turbulent motions from sparse observations?





Plenty of exciting research questions left… 👍

Thanks for Listening!

https://physicsbaseddeeplearning.org

Acknowledgements: Q. Liu, G. Kohl, B. List, L. Chen, B. Holzschuh